Cyclohexane 110-82-7 | DTXSID4021923

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.48

Global applicability domain: Inside

Local applicability domain index: 6.68e-01

Confidence level: 8.74e-01

Nearest Neighbors from the Training Set

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Cyclohexane Measured: 3.44 Predicted: 3.48 Image not found

Cycloheptane Measured: 4.00 Predicted: 4.00 Image not found

Cyclopentane
Measured: 3.00
Predicted: 2.87

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Methylcyclopentane Measured: 3.37 Predicted: 3.38 Image not found

n-Hexane Measured: 3.90 Predicted: 3.96